

K -theory on arbitrary manifolds and topological insulators

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ABSTRACT

We discuss means to study topological properties of wavefunctions in a time reversal invariant crystalline system through K -groups. The well-known methods for calculating K -groups of G -bundles over spheres are extended using earlier results in order to deal with wavefunctions defined over arbitrary manifolds following a method due to Nash. The method is used to explain the existence of surface gap less states for the topological insulator.

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1 Introduction

Topological insulators are novel band insulators invariant under time reversal possessing strong spin-orbit coupling [1]. The special surface conductivity properties of these insulators can be explained using topological arguments. We show that gapless surface states appear because of four factors. First the wavefunctions in momentum space are defined on a three torus $S^1 \times S^1 \times S^1$ due to the periodic nature of the Brillouin zone. Second, the presence of spin means the non-relativistic system has a $SU(2)$ symmetry coming from the Pauli spin matrices. Thirdly, time reversal invariance changes the $SU(2)$ symmetry to $SU(2)/\mathbb{Z}_2$ symmetry. Finally, if the spin-orbit coupling is strong enough then surface electrons can be raised to the conduction band. If these factors are present topology predicts the existence of gapless surface but not bulk states [2–4] anticipated beforehand [5, 6]. Observation of such materials [7] has enkindled expectations of discovering newer materials with unusual properties or new stable coherent quantum structures through topological studies [8]. Condensed matter systems often exhibit interesting topological features simply because they have topologically non-trivial Brillouin zones.

We will describe topological method of K -theory to explain what is observed. In order to do that some background results are required. Before we explain K -theory we point out that a variety of topological tools are available. The power of the approach we describe is that it is applicable for systems whose wavefunctions are constructed over arbitrary manifolds. Even for such systems the algebraic approach can spot topological features rather easily using two basic theorems of James and results from K -theory that we summarise.

Associating a wavefunction to every point of the Brillouin zone which we replace by an arbitrary manifold requires constructing a vector bundle over the manifold. This means smoothly gluing the wavefunctions (which are complex spinors and is a vector space) to points of the manifold. Topological methods tell us how many inequivalent ways this cannot be done. This is the problem of classifying vector bundles, for which K -theory is a standard tool. The relevance of K -theory for classifying topological insulators has been noted earlier [4, 9–12]. Our aim is to explain this in a self-contained manner. We show that a topological insulator is characterized by one or three \mathbb{Z}_2 groups in two or three dimensions, respectively. The approach adopted here was first developed by Nash [13] to classify Yang-Mills bundles over T^4 but can be easily used to classify bundles over a wide class of manifolds. This has been used to study persistent metastable currents in superfluid ^3He in its A phase in a toroidal container [14]. In view of the growing use of topological arguments in condensed matter physics it seems worthwhile to present a self-contained account of this powerful method illustrating its usefulness to classify the topological insulator.

In order to make our account reasonably self-contained we recall the constraint due to time reversal invariance for spinor systems with spin-orbit coupling in section 2. In sections 3 and 4 the basic ideas of principal bundles and K -theory, respectively, indicating their relevance in studying such systems. In section 5 we review the general method of calculating K -groups for principal bundles on tori, applying it for the present cases in section 6 before concluding in section 7 with a few remarks about the approach.

2 Time reversal symmetry

A D -dimensional crystalline system is a periodic structure specified by a lattice Λ in the D -dimensional Euclidean space, $\Lambda \subset \mathbf{R}^D$. We simplify discussion by assuming $\Lambda = \mathbf{Z}^D$, the square lattice. Denoting the inner product with $\langle \cdot, \cdot \rangle : \Lambda \times \Lambda \rightarrow \mathbf{C}$, the dual lattice

$$\Lambda^\vee = \{k \in \mathbf{R}^D | \langle k, \gamma \rangle \in 2\pi\mathbf{Z}, \forall \gamma \in \Lambda\} \quad (1)$$

is called the reciprocal lattice. Its elements k are crystal momenta, which label the irreducible representations of the Abelian group \mathfrak{T} of translations by vectors in Λ . Two crystal momenta differing by a reciprocal lattice vector correspond to the same representation. It thus suffices to consider crystal momenta k valued in the smallest domain \mathcal{B} obtained by bisecting the reciprocal lattice vectors with perpendicular planes. This is called the Brillouin zone, which is isomorphic to a torus, $\mathcal{B} \simeq T^D = \mathbf{R}^D / \Lambda^\vee$.

Electronic states, neglecting spin, of a crystalline system are taken to be the eigenfunctions can be reduced to a single particle Hamiltonian description. Such a description can come starting from a tight binding model.

$$H = -\nabla^2 + V(x), \quad (2)$$

where V is a sufficiently regular real-valued function on \mathbf{R}^D / Λ . As H is invariant under \mathfrak{T} , it possesses the same eigenfunctions as the translations in \mathfrak{T} . Introducing an orthogonal set of basis vectors in the Hilbert space \mathcal{H} underlying the irreducible representations of \mathfrak{T}

$$\Psi_n(x, k) = e^{i\langle k, \gamma \rangle} \psi_n(x, k), \quad (3)$$

$$\psi_n(x + \gamma, k) = \psi_n(x, k), \quad \gamma \in \Lambda, \quad (4)$$

called Bloch functions, the electronic states are given by a solution to the eigenvalue problem

$$H(k)\psi_n(x, k) = E_n(k)\psi_n(x, k). \quad (5)$$

The eigenvalue $E_n(k)$ of the Bloch Hamiltonian $H(k)$, called the n -th band function, is a continuous function of the crystal momentum $k \in \mathcal{B}$ for each $n = 0, 1, 2, \dots$.

Topological insulators are crystalline systems invariant under time reversal. Electronic states of such systems, in addition to being irreducible representations of \mathfrak{T} , form a representation of the finite group generated by the time reversal operator \mathcal{T} . Assuming that the time evolution of an eigenstate $\psi_n(x, k)$ of the Hamiltonian H with eigenvalue E is given by $e^{iEt}\psi_n(x, k)$, with E positive, in conformity with the time-dependent Schrödinger equation, the time reversal operator is taken to be anti-unitary, that is an endomorphism of the Hilbert space \mathcal{H} mapping the inner product to its complex conjugate. It changes the sign of the momentum and time, keeping the position of a state unaltered, that is

$$\mathcal{T} : \psi_n(x, k) \longmapsto \psi_n^*(x, -k), \quad (6)$$

where a \star denotes complex conjugation. On physical grounds a state is assumed to come back to itself up to a phase if acted on by \mathcal{T} twice, so that

$$\mathcal{T}^2 = \alpha, \quad |\alpha| = 1. \quad (7)$$

The time reversal operator \mathcal{T} is assumed to act on the Bloch Hamiltonian by conjugation as

$$\mathcal{T}H(k)\mathcal{T}^{-1} = H(-k), \quad (8)$$

The Hilbert space \mathcal{H} then correspond to a chosen representation of \mathcal{T} .

If the spin of electrons is taken into consideration, then the Hamiltonian contains terms involving spin 1/2 operators valued in a representation of the group $SU(2)$ furnished by the 2×2 Pauli matrices. The corresponding Bloch wavefunctions over \mathcal{B} , written as $\psi_n(x, k) = \begin{pmatrix} \psi_{n\uparrow}(x, k) \\ \psi_{n\downarrow}(x, k) \end{pmatrix}$, transform as vectors under the $SU(2)$, where the upper and lower components are referred to as the spin up and down states, respectively. By flipping the sign of momentum \mathcal{T} changes the sign of angular momentum. The same is assumed for spin.

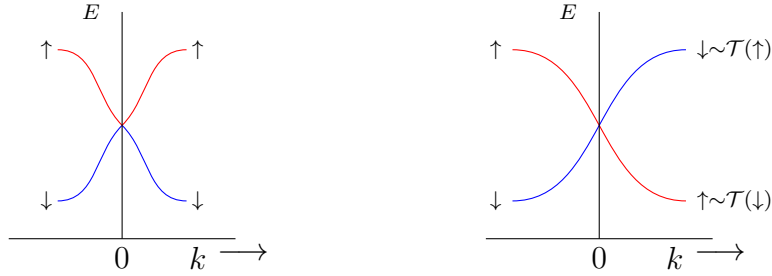


Figure 1: Osculatory (left) and intersecting (right) band functions for Kramer pairs

A consistent choice of \mathcal{T} is given by the transformation

$$\mathcal{T} : \begin{pmatrix} \psi_{n\uparrow}(x, k) \\ \psi_{n\downarrow}(x, k) \end{pmatrix} \mapsto \begin{pmatrix} \psi_{n\downarrow}^*(x, -k) \\ -\psi_{n\uparrow}^*(x, -k) \end{pmatrix} \quad (9)$$

with $\mathcal{T}^2 = -1$. The identification of wavefunctions up to a sign under \mathcal{T}^2 breaks the group $SU(2)$ acting on them to $SU(2)/\mathbb{Z}_2 \simeq SO(3)$. Thus the introduction of spin-orbit interactions allows changing the group acting on the spinor wavefunctions from being $SU(2)$ to $SU(2)/\mathbb{Z}_2$. This result plays a crucial role.

Invariance under time reversal, in general, requires the existence of a state with energy $E(-k)$ if one with $E(k)$ exists, implying thereby, that states with $E(k_0) = E(-k_0)$ at a point k_0 , called the Kramer point, are twofold degenerate, having both ψ and $\mathcal{T}\psi$ as eigenfunctions, referred to as a Kramer pair. Generically, $k_0 = 0$ is a Kramer point as well as $k_0 = \pm 1$, as these two points are identified in \mathcal{B} . A Kramer pair at $k = 0$ may be associated to states on two sides of $k = 0$ in two inequivalent ways maintaining the continuity of Bloch wavefunctions as well as the band function. This is schematically shown in Figure 1, where band functions are plotted and the spinorial components of wavefunctions are indicated.

In one configuration, shown in the diagram on the left, the spin up and down components of the Kramer pair go over respectively to the up and down components of a Bloch wavefunction on both sides, resulting into two oscillatory curves at the Kramer point. The second configuration is obtained as the

up and down components go over respectively to the up and down components on one side but to a time-reversed wavefunction on the other, with up and down components exchanged according to (9), as indicated in the diagram on the right of Figure 1. This results in two intersecting curves with distinct tangents at the Kramer point. Existence of distinct tangents mean that the band function forms a Dirac cone at this point, since the dispersion in a neighborhood of the intersection point can be brought to the form $E = \pm k$. These are the only two types of band functions that may appear in a time reversal invariant crystalline system.

3 Wavefunctions and bundles

In this section we describe Bloch wavefunctions on the Brillouin zone \mathcal{B} in terms of principal G -bundles. WE should remember that the methods we will describe are applicable for arbitrary compact manifolds although we will very often mention the three torus in our discussions. A (principal) G -bundle [15, 16] over M is built by gluing together a fixed vector space at each point of a smooth manifold M , called a *base space*. Each vector space, called a *fiber*, is acted upon linearly by a group G . The action of G is assumed to be transitive, meaning every point of a fiber F can be reached from some point in F through an action of G and there is no point held fixed by G under the action of G . The gluing procedure is best described by first covering the base space M with a collection of possibly overlapping contractible open sets $\{U_\alpha, U_\beta, \dots\}$ with a choice of vector spaces $\{F_\alpha, F_\beta, \dots\}$ on each open set, where α, β, \dots are valued in some countable index set. On an open set U_α the bundle V is simply the product of the spaces U_α and F_α . The map from V to this product space is a coordinate map ϕ_α which is said to describe the bundle V locally. If two open sets U_α and U_β overlap then the bundle V will have two coordinate descriptions in the overlapping region. A map given to link these two descriptions consistently is called a transition function. Finally, a bundle V has a projection map $\pi : V \rightarrow M$. It describes the way in which overlapping descriptions of M must be joined together to describe the global bundle space M . A G -bundle is said to be of *rank* k if the dimension of the fiber is k at every point of M . Thus the bundle is constructed by gluing together spaces, that are locally the product of one of the open sets that cover the base space M and the fiber space F . The twists and turns of the resultant bundle space are captured by the gluing procedure. The local product structure of a bundle V is called a local trivialization. Thus, a G -



Figure 2: Fiber Bundles: trivial (left) and non-trivial (right)

bundle of rank k over a smooth manifold M is a smoothly varying locally trivial family of k -dimensional vector spaces endowed with an action of G . If the bundle V can be described as the direct product of M

and a vector space F then the bundle is said to be *trivial*. As an example, if M is a circle S^1 and the fiber at each point is an oriented line, then the lines can be glued together maintaining their orientations to form a cylinder, which is a trivial bundle, or with a twist, changing orientations along the circle such that the orientation is reversed upon traversing the circle once, yielding a Möbius strip, which is not trivial. These are schematically shown in Figure 2. Over a given base space vector bundles are topologically classified up to isomorphism. Two bundles on M are isomorphic if on each open set U_α the vector spaces corresponding to these are isomorphic.

Let us discuss the connection between the time reversal invariant systems and G -bundles. A Bloch wavefunction $\psi(x, k)$ is an element of the Hilbert space \mathcal{H} which varies over the Brillouin zone \mathcal{B} parametrized by k . Hence the group of endomorphisms of \mathcal{H} , which form a module over \mathcal{H} varies over \mathcal{B} too. As the wavefunctions transform under an $SO(3) \simeq SU(2)/\mathbf{Z}_2$, as shown before, we are led to considering $SO(3)$ -bundles over the torus \mathcal{B} . This corresponds to considering wavefunctions associated to two types of band functions discussed above. Whether or not the twisting can occur in a real system depends on the details of the Hamiltonian. The geometric picture we consider only classifies the different possibilities, of which there are but two, the first corresponding to a conventional insulator while the second to a topological one.

Since the isomorphism of vector spaces on an open set is required to be consistent with the action of the group G on the fibers, a classification scheme for vector bundles depends on properties of G . The standard procedure is to determine the homotopy class of maps from the base space M of V to the classifying space BG associated with G . Homotopy properties of BG are known. In a homotopic classification two maps belong to the same class if they can be continuously deformed into each other and to different classes otherwise. Fortunately we do not need to get into the details of the space BG since for vector bundles over a D -sphere S^D the homotopy classes that need be computed depend only on the fiber group G . We also outline how K -theory fits in within this scheme. In order to classify vector bundles over a base space that is not a sphere we need to master a few simple specialized methods. This mastery is necessary as the problem of classifying topological insulators is, as we show, the same as the problem of classifying vector bundles over tori. We thus first explain how the K -theoretic method can be used to classify vector bundles over arbitrary base manifolds and then use this general method to classify the topological insulator.

4 K -theory

K -theory may be thought of as a generalized cohomology theory used to classify vector bundles [16, 17]. This means that it satisfies all the properties required for cohomology theory except the axiom of dimensions. A very readable account of these matters is given in Nash [17] The method directly works with vector bundles and spots twists from the Abelian group structure introduced for adding bundles. The Abelian group operation between bundles starts by defining addition of bundles over the same base space simply as the usual addition of vector spaces. The fiber of the sum of two vector bundles on any open set of the base space is taken to be the sum of fibers of the summands on the same open set. A trick analogous to the definition of integers from natural numbers then leads to the notion of subtraction of

bundles. The idea is very simple. Subtraction of numbers have the property $7 - 5 = 9 - 7 = \dots$. Thus we use this result and first write it as $a - b = c - d$ and define subtraction as $a + d = c + b \rightarrow a - b = c - d$. This yields an Abelian group, known as the K -group, with vector bundles as its elements and addition of bundles as the group operation, its inverse operation being the subtraction. This is the K -group of the bundle. Topological information is fed into the structure by stating that a pair of vector bundles are isomorphic if they differ by the addition of a trivial bundle of appropriate rank, the latter taken to play the role identity like zero in the group of integers. A vector bundle $V^{(k)}$ of rank k on a manifold M of dimension D is said to be in the *stable range* if $k > D$. Usefulness of the K -group comes from

Theorem 4.1 (Nash [17]). If a vector bundle $V^{(k)}$ is in the stable range, then there is an isomorphism between the vector bundles $V^{(k)}$ and $V^m + I^{(k-m)}$ with $m < k$, where $V^{(m)}$ is a vector bundle of rank m and $I^{(k-m)}$ is a trivial bundle of rank $(k - m)$ both defined over the base space M . We write $V^{(k)} = V^{(m)} + I^{(k-m)}$.

This means that the totality of topological information of a vector bundle of a sufficiently large rank is effectively encoded in a vector bundle of lower rank. This allows for the following equivalence relation between vector bundles.

Definition 4.1. Two vector bundles V_1 and V_2 are equivalent if $V_1 + I^\ell = V_2 + I^r$, where ℓ and r are positive integers. We write $V_1 \sim V_2$.

We have the convenient

Lemma 4.1. For vector bundles V_0, V_1 and V_2 , if $V_1 + V_0 = V_2 + V_0$, then $V_1 \sim V_2$.

The proof is based on the fact [17] that for a reasonable manifold M it is always possible to find for a given vector bundle V_0 on M , a bundle V'_0 , such that $V_0 + V'_0 = I$, I being a trivial bundle. Thus $V_1 + V_0 = V_2 + V_0$ implies $V_1 + V_0 + V'_0 = V_2 + V_0 + V'_0$, or $V_1 + I = V_2 + I$, that is $V_1 \sim V_2$.

This equivalence relation partitions the set of vector bundles on a fixed base space into equivalence classes, which generalizes the isomorphism classes in K -theory. The usual notion of isomorphism follows by considering vector bundles of equal ranks. From now on a vector bundle will be taken to refer to a representative of the equivalence class to which it belongs. We have considered addition of vector bundles and their equivalence through the addition of a trivial bundle. Let us now discuss the subtraction. The notion of subtraction of vector bundles parallels a particular feature of subtraction of natural numbers. Let us consider two pairs of natural numbers $\{v_1, v_2\}, \{v'_1, v'_2\}$ and write their pairwise differences as the ordered pairs, namely, $(v_1, v_2) = v_1 - v_2$ and $(v'_1, v'_2) = v'_1 - v'_2$. If the differences are equal, that is $(v_1, v_2) = (v'_1, v'_2)$, then we can also write $v_1 + v'_2 = v'_1 + v_2$, using the usual properties of subtraction as the inverse of addition for natural numbers, or, equivalently,

$$v_1 + v'_2 + v = v_2 + v'_1 + v \quad (10)$$

where v is an arbitrary natural number. Reasoning backwards, subtraction of two natural numbers (s, t) is now defined as the ordered pair so that $(v_1, v_2) = (v'_1, v'_2)$ for two pairs of natural numbers implies equation (10).

This notion is used to define the subtraction of vector bundles. Given a pair of vector bundles V_1 and V_2 on M their difference, also considered to be a vector bundle on M , is defined to be an ordered pair (V_1, V_2) , such that if $(V_1, V_2) = (V'_1, V'_2)$ for two pairs of vector bundles, then

$$V_1 + V'_2 + V = V_2 + V'_1 + V, \quad (11)$$

for any vector bundle V over M . The difference (V_1, V_2) is also called a *virtual bundle* and denoted $V_1 - V_2$, with *virtual dimension* of $V_1 - V_2$ defined as the difference between the ranks of the individual bundles V_1 and V_2 . Let us point out that the virtual dimension can be negative; it is zero if both the bundles have the same rank. As alluded to above, this notion of addition and subtraction of vector bundles endow the set of equivalence class of vector bundles with the structure of an Abelian group, known as the K -group.

5 Computing K -groups

In this section we discuss the computation of K -groups of G -bundles on tori in general. Let us first recall that two spaces are said to be *homeomorphic* if they are mapped to each other by a continuous one-to-one and onto mapping with a continuous inverse. Let us also recall that a sequence of Abelian groups

$$0 \longrightarrow A \xrightarrow{f} B \xrightarrow{g} C \longrightarrow 0 \quad (12)$$

is said to be *exact* if the image of the group A into the group B under the injective mapping f is mapped to the identity element of the group C by the surjective mapping g , as illustrated in Figure 3. This is a

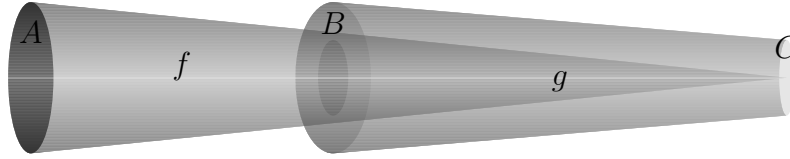


Figure 3: Pictorial presentation of the exact sequence (12)

manner of expressing the fact that C is same as B modulo A , which is shrunk to a point in C .

To compute K -groups of vector bundles on tori (or more general manifolds) in terms of vector bundles on spheres the tori (or more general manifolds) need be described in terms of spheres. We start by introducing certain combinations of topological spaces. Let X and Y be two (topological) spaces with base-points, that is each one has one point marked as distinguished, which we denote by x_0 and y_0 , respectively. We will see that the K groups of spheres are related to homotopy groups. These require a fixed base point. In the space $x \times Y$ the fixed points are a pair, one belonging to X , one belonging to Y . In order to tackle this problem the idea is to smash these two points together. This done by a quotient construction which we now describe. We start with the *Cartesian product* $X \times Y$ of X and Y is defined to be the set of ordered pairs of points from X and Y , namely

$$X \times Y = \{(x, y) | x \in X, y \in Y\}. \quad (13)$$

For example, a two-torus is (homeomorphic to) the Cartesian product to two circles, $T^2 \simeq S^1 \times S^1$, with $X = S^1$ and $Y = S^1$, as depicted in Figure 4. The *wedge sum* $X \vee Y$ is the disjoint union of X and Y

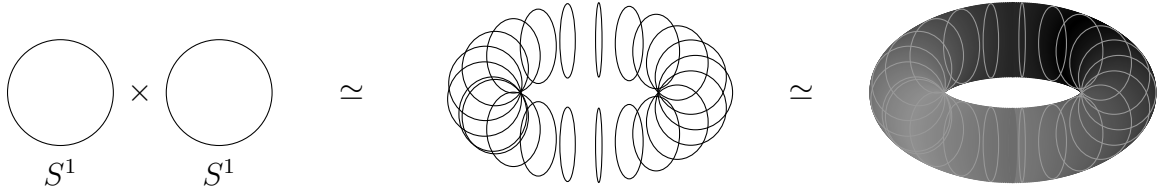


Figure 4: Cartesian product of circles: two-torus

but with the base-points identified. That is

$$X \vee Y = X \sqcup Y / (x_0 \sim y_0). \quad (14)$$

For example, the wedge sum of two circles is (homeomorphic to) a figure eight as indicated in Figure 5. The *smash product* $X \wedge Y$ of X and Y is defined as their Cartesian product with the subsets $(x_0, Y) = \{(x_0, y) | y \in Y\}$ and $(X, y_0) = \{(x, y_0) | x \in X\}$ identified. Thus

$$X \wedge Y = X \times Y / ((x_0, y) \sim (x, y_0)), \quad \forall x \in X, \forall y \in Y. \quad (15)$$

The subsets X and Y of $X \times Y$ can be looked upon as the subspaces $X \times \{y_0\}$ and $\{x_0\} \times Y$, respectively, intersecting at x_0, y_0 , which is taken to be the base-point of $X \times Y$. Thus their union can be identified with the wedge sum $X \vee Y$. Hence the smash product can be expressed as a quotient

$$X \wedge Y = (X \times Y) / (X \vee Y), \quad (16)$$

which can also be described as the sequence of mappings

$$0 \longrightarrow X \vee Y \longrightarrow X \times Y \longrightarrow X \wedge Y \longrightarrow 0, \quad (17)$$

where the first map is injective taking a point, denoted 0, to the basepoint of $X \vee Y$, while the last map is surjective collapsing the entire space $X \wedge Y$ to a point, as depicted in Figure 3.

The smash product of two circles is (homeomorphic to) a sphere, S^2 . To see this we first “open up” one circle in $S^1 \times S^1$ to an interval whose end points are to be identified. While for $S^1 \wedge S^1$ introduce an interval between the two circles that form originally formed a figure eight. The end points of this interval

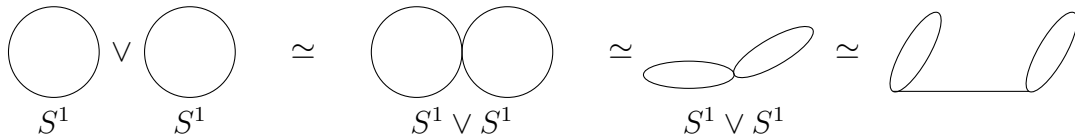


Figure 5: Wedge sum of two circles



Figure 6: Alternative view of Cartesian product of two circles

identified by shrinking the interval to a point gives back the figure eight. For the Cartesian product $S^1 \times S^1$ this is depicted in Figure 6, where the radii of the circles along the interval is varied, decreasing from the center towards the end on both sides, without affecting the topology of the configuration. Upon identification of the end points it becomes the torus of Figure 4. Similarly, the figure eight wedge sum $S^1 \vee S^1$ is opened up as indicated in the last diagram of Figure 5 with the two circles placed at the end points of an interval, which is contractible to a point. The figure eight is recovered upon identification of the end points of the interval. We can now describe the quotient $S^1 \wedge S^1$ pictorially as the quotient of these two pictures, shrinking the interval in Figure 6 with the circles at its end points brought together to a point due to the identification by the configuration in the last diagram of Figure 5. This yields a sphere S^2 as indicated in Figure 7. Coming back to the computation of K -groups, we use a result of K -theory which proves that corresponding to sequence of maps between spaces $X \vee Y, X \times Y, X \wedge Y$ that we described there is associated an exact sequence of the K -groups with the linking homomorphisms for the groups in reverse order to those introduced for the spaces. Thus, we have an exact sequence of K -groups

$$0 \longrightarrow K(X \wedge Y) \longrightarrow K(X \times Y) \longrightarrow K(X \vee Y) \longrightarrow 0 \quad (18)$$

is associated to the sequence of maps introduced earlier (17). Here and in the following we ignore the contribution of points, which are zero-dimensional, to the K -group thus restricting attention to the *reduced* K -group only, while continue denoting it with K . Since the group operation of the K -group

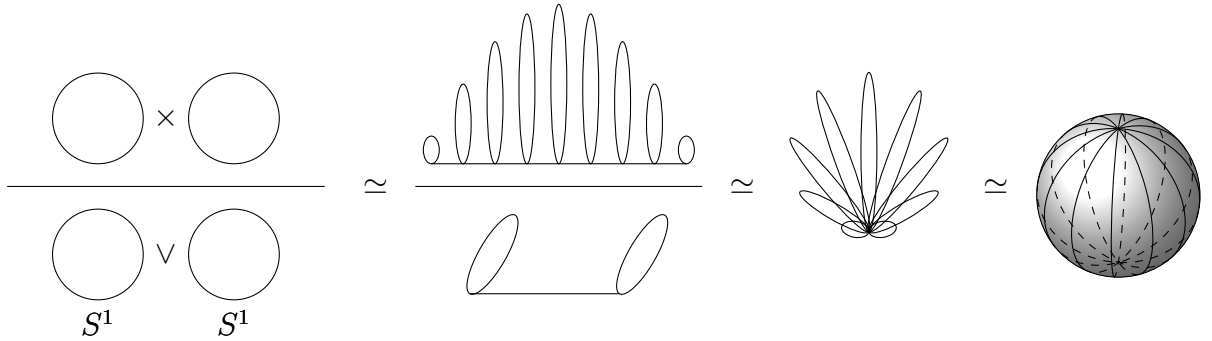


Figure 7: Smash product of two circles as a quotient

addition, as described in the previous section, it follows that

$$K(X \times Y) = K(X \wedge Y) + K(X \vee Y). \quad (19)$$

But for the wedge sum we have

$$K(X \vee Y) = K(X) + K(Y). \quad (20)$$

Combining these we have the

$$K(X \times Y) = K(X \wedge Y) + K(X) + K(Y). \quad (21)$$

The scope of K -theory is rather general in that it deals with bundles of arbitrary rank. The definition of K -groups can be restricted to G -bundles over spaces. The K -group of G -bundles over X will be denoted as $K_G(X)$. The computation of K -groups on spheres is facilitated by their relation with homotopy groups of the structure group of the vector bundles. The reduced K -group of a G -bundle on a D -dimensional sphere is given by

$$K_G(S^D) = \pi_{D-1}(G), \quad (22)$$

where $\pi_n(G)$ denotes the n -th homotopy group of G . Let us sketch the proof of this for completeness. A sphere S^D can be represented topologically by its cover with two contractible spaces U_1 and U_2 . These spaces overlap to form the topological space S^{D-1} . As U_1 and U_2 are contractible spaces homeomorphic to \mathbf{R}^D , bundles on them are trivial, that is direct products, $U_1 \times F$ and $U_2 \times F$, respectively, where F is the fiber space on which the group structure group G acts. The nature of bundles on S^D thus depends on the way of gluing the trivial bundles on U_1 and U_2 together. This in turn depends on the homotopy properties of the map from the intersection of U_1 and U_2 to G , namely, $S^{D-1} \simeq U_1 \cap U_2 \rightarrow G$. But this is just $\pi_{D-1}(G)$, by definition.

6 K -groups for time reversal invariant systems

We proceed to compute the reduced K -groups of $G = SO(3)$ -bundles on the toroidal Brillouin zone \mathcal{B} for a time reversal invariant crystalline system. For two- and three-dimensional systems $\mathcal{B} = T^2$ and $\mathcal{B} = T^3$, respectively.

In the two-dimensional case by the identification of the Cartesian product of two circles with a two-torus and the smash product of two circles with a two sphere, we obtain,

$$\begin{aligned} K_G(T^2) &= K_G(S^1 \times S^1) \\ &= K_G(S^1 \wedge S^1) + K_G(S^1) + K_G(S^1) \\ &= K_G(S^2) + 2K_G(S^1), \end{aligned} \quad (23)$$

where the notation $K(X) + K(X) = 2K(X)$ is used for K -groups in analogy with the natural numbers. Next, using (22) equation (23) yields

$$K_G(T^2) = \pi_1(G) + 2\pi_0(G), \quad (24)$$

where $G = SO(3)$. Ignoring the last term in reduced K -theory we then obtain

$$K_{SO(3)}(T^2) = \pi_1(SO(3)) = \mathbf{Z}_2. \quad (25)$$

The two classes in the K -group represent the two types of bundles corresponding to the osculating and intersecting band functions discussed in section 2.

For the three-dimensional system we compute the reduced K -group of $SO(3)$ -bundles on $T^3 = S^1 \times S^1 \times S^1$. Defining $Y = S^1 \times S^1 \simeq T^2$ we use (21) to obtain

$$\begin{aligned} K_G(T^3) &= K_G(S^1 \times Y) \\ &= K_G(S^1 \wedge Y) + K_G(S^1) + K_G(Y) \\ &= K_G(S^1 \wedge Y) + \pi_0(G) + K_G(T^2) \\ &= K_G(S^1 \wedge Y) + \pi_1(G), \end{aligned} \quad (26)$$

where we have used the results for the two-torus and ignored π_0 . In order to calculate $K_G(S^1 \wedge Y)$ we need the

Theorem 6.1 (James [18]). The r -th Betti number b_r of Y contributes a $K_G(S^{r+1})$ to the K -group of the wedge sum $K_G(S^1 \wedge Y)$.

This arises from the fact that the r -th Betti number counts the number of r -th homology cycles of Y which are r -spheres. These contribute to the K -group in one higher dimension due to the extra S^1 . Betti numbers of $Y \simeq T^2$ are $b_0 = 1, b_1 = 2, b_2 = 1$. Hence

$$K_G(S^1 \wedge Y) = K_G(S^1) + 2K_G(S^2) + K_G(S^3). \quad (27)$$

We thus have, up to π_0 of circles and spheres,

$$K_G(T^3) = 3\mathbf{Z}_2 + K_G(S^3) \quad (28)$$

in reduced K -theory. The last term requires special treatment not being in the stable range. We need the following

Theorem 6.2 (James & Thomas [19, Th. 1.6]). The map $[T^3, BSO(3)] \longrightarrow [T^3, BSO] = K(T^3)$ is injective, and under this map the elements of $[T^3, BSO(3)]$ correspond to the subgroup of $K(T^3)$ with vanishing third Steifel Whitney class.

Here $T^3 = S^1 \times S^1 \times S^1$ and the Steifel Whitney class $H^3(S^3, \mathbf{Z}_2) = \mathbf{Z}_2$ is non-zero. Hence $K(T^3)$ is the trivial group. Thus

$$K_{SO(3)}(T^3) = 3\mathbf{Z}_2, \quad (29)$$

which agrees with previous results [4, 9, 10].

In section 2 we proved the existence of Dirac cones as a consequence of gap-less states appearing as band functions intersect. Let us briefly discuss how the appearance of gap-less states are understood from K -theory analysis. This is done by including an $SU(2)/\mathbf{Z}_2 \simeq SO(3)$ -connection because of time

reversal symmetry. We cannot use $SO(3)$ directly as $SO(3)$ does not act on spinors. The index of the Dirac operator D , which acts on smooth sections of the $SU(2)/\mathbf{Z}_2$ -bundle on the torus \mathcal{B} , is defined as

$$\begin{aligned}\text{ind } D &= \text{ch}(\ker D - \text{coker } D) \\ &= \text{ch}(\ker D) - \text{ch}(\text{coker } D),\end{aligned}\tag{30}$$

where the Chern character map from the K -group of a space to its rational cohomology, namely,

$$\text{ch} : K(X) \rightarrow H^\bullet(X, \mathbb{Q})\tag{31}$$

is used to map the virtual bundle $\ker D - \text{coker } D$ in $K_G(\mathcal{B})$ to $H^\bullet(\mathcal{B}, \mathbb{Q})$. Since the K -group as computed above, is non-zero, either the kernel or its dual, the cokernel, of D is non-void, implying the existence of zero modes, alias, gap-less states, at some point of \mathcal{B} .

7 Conclusion

We have outlined a general method of calculating K -groups for vector bundles over arbitrary base manifolds and have illustrated the method for the $SO(3)$ -bundles on two- and three-dimensional tori. We have explained the relevance of K -groups for time reversal invariant crystalline systems, for example, topological insulators. The computation of K -groups are facilitated by reducing the calculation of K -groups for spaces $S \wedge Y$ in terms of the K -group of spheres [18, 19]. Results thus obtained are consistent with previous results and clarify the occurrence of a trinity of \mathbf{Z}_2 groups rather than a possible quartet. The usefulness of K -theory lies in that it allows to bring out topological properties of bundles on tori, $S^1 \times S^1 \times S^1$ in a purely algebraic manner. Let us note that had the structure group of the bundle been $SU(k)$ for any k , *i.e.* had we have to deal with complex bundles, the K -groups would have been trivial [17]. Thus the time reversal symmetry which breaks $SU(2)$ to $SO(3)$ is essential in that there would have been no topological reason for the stability of the topological insulators in want of this symmetry. Based on the analysis presented we can give an intuitive account explaining the role strong spin-orbit interaction and time reversal invariance play in the formation of a Dirac point in the topological insulator. Suppose a spinor system is described by a non relativistic Hamiltonian, without spin-orbit coupling. We further suppose that the system has a band gap and there are no electrons present in the conduction band. Time reversal symmetry for this system replaces ψ by ψ^* with fibre group $SU(2)$. Now introduce a strong spin-orbit interaction term. This has two effects. It can shift electrons to the conduction band and now the presence of the $\sigma.L$ term changes the operation of time reversal to the replacement of $\psi \rightarrow \sigma_2 \psi^*$. The effect of this as we saw was changing the fibre group from $SU(2)$ to $SU(2)/\mathbf{Z}_2$ the \mathbf{Z}_2 factor produced a non zero K -group which implied via the index theorem a gap-less point. An implication of this sketch is that if an interaction term is introduced with a finite subgroup symmetry of $SU(2)$ so that the fibre group gets modified from $SU(2)$ to $SU(2)/G$ then the system will have a non-trivial K -group and if the interaction introduced can raise electrons to the conduction band of the system then topology dictates that the system has to have a gap-less point.

The K -groups can be multiplied, forming a ring. While only the case of a single Dirac point has been dealt with above, multiple Dirac points can be treated similarly through a tensor product of vector

bundles, whose K -group is the product of the K -groups of the factors, one for each Dirac point. This immediately implies triviality of K -groups for an even number of Dirac points and non-triviality of the same for an odd number as the product of an even number of \mathbf{Z}_2 's is trivial but is that of an odd number of \mathbf{Z}_2 's is not.

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